Lecture 3: Adaptive Construction of Response Surface Approximations for Bayesian Inference

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Outline

- Introduction.
- A few words about validation.
- Application of GOEE to Bayesian Inference.
- Numerical examples.

Introduction

Questions pertaining to validation

Is the model any good?
Is the model a good model?
How good is the model?

If one wants to be philosophical...

What is a good model?

Before answering those questions, one must have an objective in mind.

Quantities of interest:

Specific objectives that can be expressed as the target outputs of a model (mathematically, they are often defined by functionals of the solutions).

Examples:

$$Q(u) = u(x)$$
$$Q(u) = \int u(x)dx$$

Some Definitions:

Verification:

The process of determining the accuracy with which a computational model can produce results deliverable by the mathematical model on which it is based.
$\Rightarrow$ **Code and Solution Verification**

Validation:

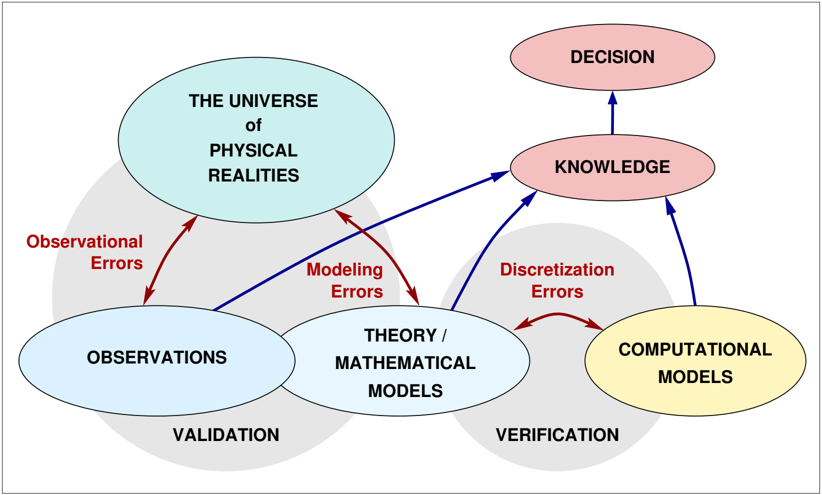
The process of determining the accuracy with which a model can predict observed physical events (or the important features of a physical reality).

P. Roache (2009): “The process of determining the degree to which a model (and its associated data) is an accurate representation of the real world from the perspective of the intended uses of the model”.

Uncertainty Quantification:

The process of determining the degree of uncertainty in the prediction of the QoI. Typically, the degree of uncertainty is related to the probability distribution for the QoI.

Paths to Knowledge



Oden, Moser, and Ghattas, SIAM News, (Nov. 2010)
Oden and Prudhomme, IJNME (Sept. 2010)

Control of Errors

Errors are all a matter of comparison!

- Code Verification: Using the method of “manufactured solutions”, for example, we can easily compare the computed solution with the manufactured solution.
- Solution Verification: In this case, the solution of the problem is unknown and one can use convergence (uniform or adaptive methods) to assess the accuracy of the approximate solutions.
- Calibration Process: Comparison of observable data with model estimates of the observables.
- Validation Process: The main idea behind validation is to know whether a model can be used for prediction purposes.

$\Rightarrow$ What should we compare in this case?

Validation Process

1. Calibration:

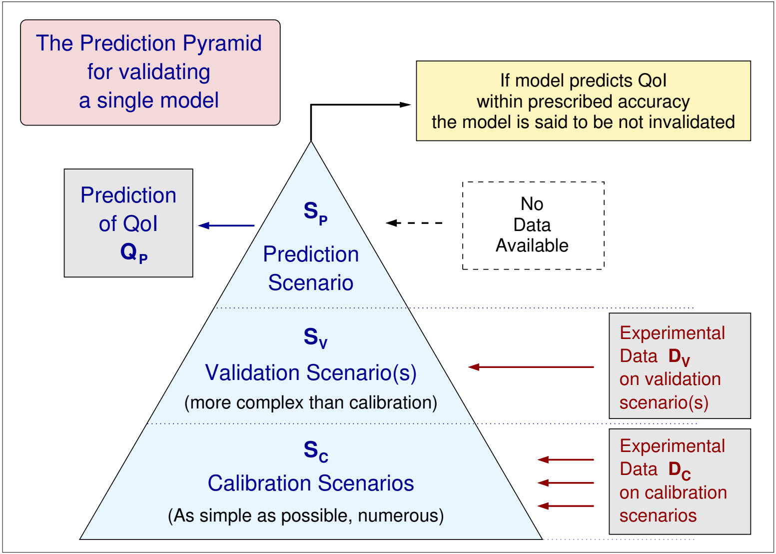
   Identification of values of parameters of a model designed to bring model results into agreement with measurements.

2. Validation:

   The process of determining the accuracy with which a model can predict observed physical events (or the important features of a physical reality).

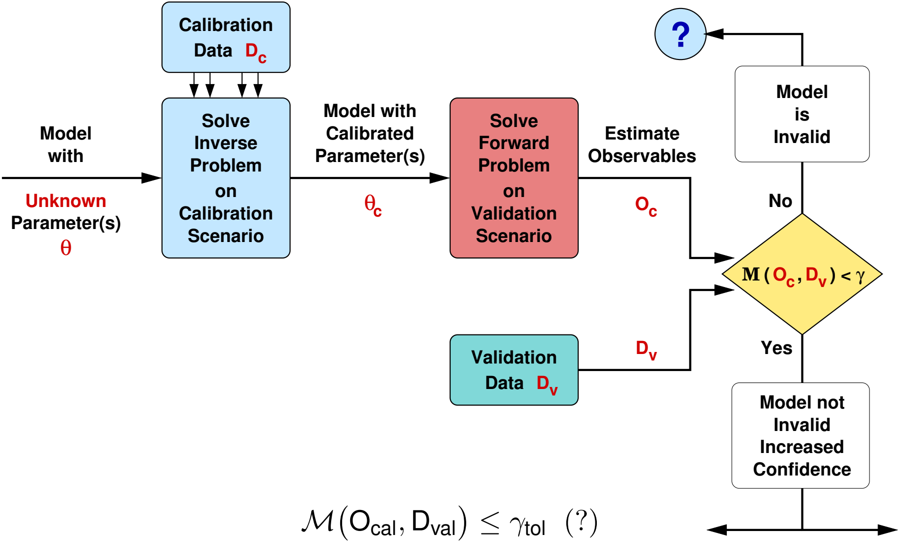
3. Prediction:

   The forecast of an event (a predicted event cannot be measured or observed, for then it ceases to be a prediction).



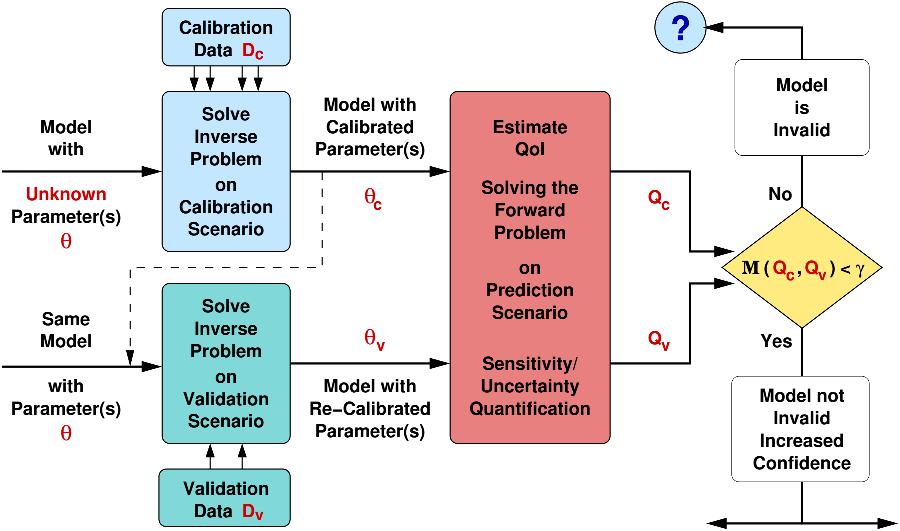
The Validation Pyramid

Classical Approach for Validation



$$\mathcal{M}\left(O_{cal}, D_{val}\right) \leq \gamma_{tol} \quad (?)$$

Proposed Validation Process (2009)



$$\mathcal{M}\left(Q_{cal}, Q_{val}\right) \leq \gamma_{tol} \quad (?)$$

Validation process requires detailed planning:

1. **Description of goals:** Describe background and goals of the predictions. Clearly define the quantity (or quantities) of interest.
2. **Modeling:** Write mathematical equations of selected model(s), list all parameters that are necessary to solve the problem, as well as assumptions and limitations of the model(s),
3. **Data collection:** Collect as many data as possible from literature or available sources (data should include, if available, the statistics).
4. **Sensitivity analysis:** Quantify the sensitivity of QoI with respect to parameters of the model. Rank parameters according to their influence.
5. **Calibration experiments:** Provide description of scenario (as precisely as possible), observables and statistics, prior and likelihood of the parameters to be calibrated.
6. **Validation experiments:** Provide same as above + clearly state assumption to be validated.

Morgan & Henrion's "Ten Commandements" (1990)*

In relation to quantitative risk and policy analysis

1. Do your homework with literature, experts and users.
2. Let the problem drive the analysis.
3. Make the analysis as simple as possible, but no simpler.
4. Identify all significant assumptions.
5. Be explicit about decision criteria and policy strategies.
6. Be explicit about uncertainties.
7. Perform systematic sensitivity and uncertainty analysis.
8. Iteratively refine the problem statement and the analysis.
9. Document clearly and completely.
10. Expose to peer review.

* Extracted from D. Vose, "Risk Analysis: A Quantitative Guide" (2008)

A systematic approach to the planning and implementation of experiments (Chapter 1 - Section 2)

In Wu & Hamada “Experiments, Analysis, and Optimization” (2009)

1. State objective.
2. Choose response.
3. Choose factors and levels.
4. Choose experimental plan.
5. Perform the experiment.
6. Analyze the data.
7. Draw conclusions and make recommendations:

   . . . the conclusions should refer back to the stated objectives of the experiment. A confirmation experiment is worthwhile for example, to confirm the recommended settings. Recommendations for further experimentation in a follow-up experiment may also be given. For example, a follow-up experiment is needed if two models explain the experimental data equally well and one must be chosen for optimization.

Planning

- Planning is a cumbersome and time-consuming process.
- Planning of validation processes involves many choices that eventually need to be carefully checked.

Choices are made about:

- Physical models
- Quantities of interest and surrogate quantities of interest
- Experiments for calibration and validation purposes
- Data sets to be used in calibration and validation
- Prior pdf and likelihood function
- Probabilistic models . . .

Our preliminary experiences with validation has revealed that many “sanity checks” need to be added within the proposed validation process.

Our objective is to develop a suite of tools to systematically verify the correctness of each stage of the validation process.

Adaptive Response Surface for Parameter Estimation

Objective

The main objective here is to develop a methodology based on response surface models and goal-oriented error estimation for efficient and reliable parameter estimation in turbulence modeling.

Bayesian inference for RANS using surrogate models

Efficient Bayesian inference: Approximate response surface models can be used to reduce the computational cost of the process.

- Ma and Zabaras, 2009.
- Li and Marzouk, 2014;
  Marzouk and Xiu, 2009;
  Marzouk and Najm, 2009.

UQ for RANS models: Uncertainty in the RANS model parameters is a known issue in the turbulence community, but quantifying the effect of this uncertainty is seldom analyzed in the computational fluid dynamics literature.

- Cheung et al., 2011.
- Oliver and Moser, 2011.

Fully developed incompressible channel flow

Mean flow equations: $\boldsymbol{u} = \boldsymbol{U} + \boldsymbol{u}'$

$$\begin{cases} \dfrac{DU_i}{Dt} = -\dfrac{1}{\rho}\dfrac{\partial P}{\partial x_i} + \dfrac{\partial}{\partial x_j}\left(\nu \dfrac{\partial U_i}{\partial x_j} - \overline{\boldsymbol{u}_i'\boldsymbol{u}_j'}\right) \\ \nabla \cdot \boldsymbol{U} = 0 \end{cases}$$

Eddy viscosity assumption:

$$\overline{\boldsymbol{u}_i'\boldsymbol{u}_j'} = -\nu_T \left(U_{i,j} + U_{j,i}\right)$$

Channel equations: assuming homogeneous turbulence in x

$$\frac{\partial}{\partial y}\left((\nu + \nu_T)\frac{\partial U}{\partial y}\right) = 1, \quad y \in (0, H)$$

[1] Durbin and Petterson Reif, 2001; Pope, 2000

Spalart-Allmaras (SA) model

Eddy viscosity is given by:

$$\nu_T = \tilde{\nu} f_{v1}, \qquad f_{v1} = \chi^3/(\chi^3 + {c_{v1}}^3), \qquad \chi = \tilde{\nu}/\nu$$

where $\tilde{\nu}$ is governed by the transport equation

$$\frac{D\tilde{\nu}}{Dt} = \mathcal{P}_{\tilde{\nu}}(\kappa, c_{b1}) - \varepsilon_{\tilde{\nu}}(\kappa, c_{b1}, \sigma_{\mathsf{SA}}, c_{w2}) + \frac{1}{\sigma_{\mathsf{SA}}}\left[\frac{\partial}{\partial x_j}\left((\nu + \tilde{\nu})\frac{\partial \tilde{\nu}}{\partial x_j}\right) + c_{b2}\frac{\partial \tilde{\nu}}{\partial x_j}\frac{\partial \tilde{\nu}}{\partial x_j}\right]$$

with

- $P_{\tilde{\nu}}$ = production term
- $D_{\tilde{\nu}}$ = wall destruction term

Parameter Values			
κ	0.41	c_{b2}	0.622
c_{b1}	0.1355	c_{v1}	7.1
σ_{SA}	2/3	c_{w2}	0.3

[1] Allmaras, Johnson, and Spalart, 2012; Oliver and Darmofal, 2009

Forward model: Find U and $\tilde{\nu}$ such that

$$\begin{cases} 1 = \dfrac{\partial}{\partial y}\left((\nu + \nu_T(c_{v1}))\dfrac{\partial U}{\partial y} \right) \\ 0 = \mathcal{P}_{\tilde{\nu}}(\kappa, c_{b1}) - \varepsilon_{\tilde{\nu}}(\kappa, c_{b1}, \sigma_{\mathsf{SA}}, c_{w2}) + \dfrac{1}{\sigma_{\mathsf{SA}}}\dfrac{\partial}{\partial y}\left[\left((\nu + \tilde{\nu})\dfrac{\partial \tilde{\nu}}{\partial y} \right) + c_{b2}\left(\dfrac{\partial \tilde{\nu}}{\partial y} \right)^2 \right] \end{cases}$$

Boundary conditions:

$$U(0) = 0, \quad \partial_y U(H) = 0, \quad \tilde{\nu}(0) = 0, \quad \partial_y \tilde{\nu}(H) = 0$$

Weak formulation:

Find $(U, \tilde{\nu}) \in \mathcal{V}$ s.t. $\quad \mathcal{B}((U, \tilde{\nu}); (V, \mu)) = \mathcal{F}(V, \mu), \quad \forall (V, \mu) \in \mathcal{V}$

Quantity of interest and adjoint problem:

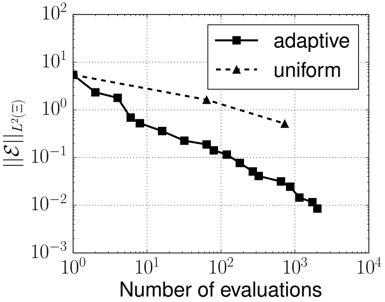
Find $(Z, \zeta) \in \mathcal{V}$ s.t.

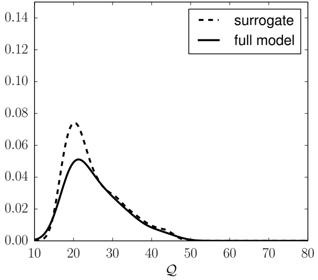
$$\mathcal{B}'((U, \tilde{\nu}); (Z, \zeta), (V, \mu)) = Q(V, \mu) = \int_0^H V \, dy \quad \forall (V, \mu) \in \mathcal{V}$$

Adaptive Response Surface

- Uniform priors for all parameters with range $(0.5, 1.5)$ times nominal value (e.g. $\kappa \sim \mathcal{U}(0.205, 0.615)$)
- Adapted expansion order (after 17 iterations):

κ	c_{b1}	σ_{SA}	c_{b2}	c_{v1}	c_{w2}
6	3	3	1	2	2





Bayesian inference

Bayes rule:

$$\boxed{p(\boldsymbol{\xi}|\boldsymbol{q}) = \frac{L(\boldsymbol{\xi}|\boldsymbol{q})\, p(\boldsymbol{\xi})}{p(\boldsymbol{q})}} \quad \text{where} \quad \begin{cases} \boldsymbol{q} \in \mathbb{R}^n & = \text{Calibration data} \\ L(\boldsymbol{\xi}|\boldsymbol{q}) & = \text{Likelihood} \\ p(\boldsymbol{\xi}) & = \text{Prior} \\ p(\boldsymbol{\xi}|\boldsymbol{q}) & = \text{Posterior} \end{cases}$$

Model selection:

- Set of models $\mathcal{M} = \{M_1, M_2, \ldots, M_n\}$
- Posterior plausibility = $p(M_i|\boldsymbol{q}, \mathcal{M})$
- Likelihood =
$$E(M_i|\boldsymbol{q}, \mathcal{M}) := p(\boldsymbol{q}|M_i, \mathcal{M}) = \int_{\Xi} p(\boldsymbol{q}|\boldsymbol{\xi}, M_i, \mathcal{M}) p(\boldsymbol{\xi}|M_i, \mathcal{M})\, d\boldsymbol{\xi}$$

$$\boxed{p(M_i|\boldsymbol{q}, \mathcal{M}) \propto E(M_i|\boldsymbol{q}, \mathcal{M})\, p(M_i|\mathcal{M})}$$

[1] Calvetti and Somersalo, 2007; Jaynes, 2003; Kaipio and Somersalo, 2005

Calibration data:

- Data is obtained from direct numerical simulation (DNS) [1]
- Mean velocity measurements were taken at $Re_\tau = 944$ and $Re_\tau = 2003$

Uncertainty models:

- Three multiplicative error models

$$\langle u \rangle^+ (z;\xi) = (1 + \boldsymbol{\epsilon}(z;\xi)) U^+(z;\xi)$$

  - independent homogeneous covariance
  - correlated homogeneous covariance
  - correlated inhomogeneous covariance

- Reynolds stress model

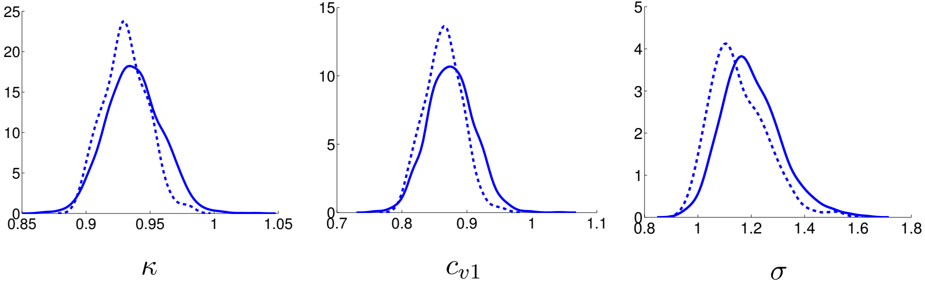
$$\left\langle \boldsymbol{u}_i' \boldsymbol{u}_j' \right\rangle^+ (z;\xi) = T^+(z;\xi) - \boldsymbol{\epsilon}(z;\xi)$$

[1] Del Alamo et al., 2004; Hoyas and Jiménez, 2006

Numerical Results

Independent homogeneous covariance:

$$\langle u\rangle^{+}(z;\xi) = (1+\boldsymbol{\epsilon}(z;\xi))U^{+}(z;\xi)$$
$$\left\langle \boldsymbol{\epsilon}(z)\boldsymbol{\epsilon}(z')\right\rangle = \sigma^2\delta(z-z')$$

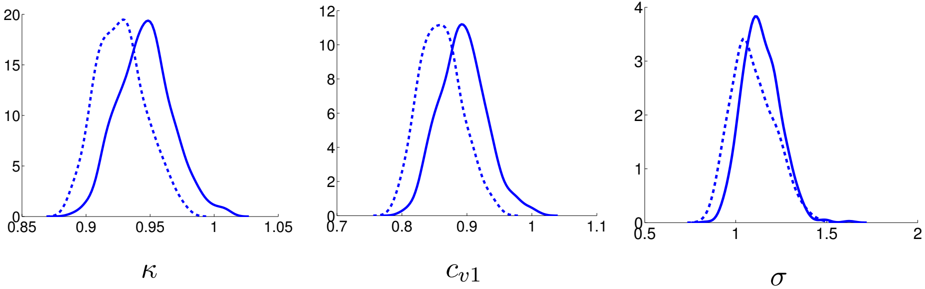


Numerical Results

Correlated homogeneous covariance:

$$\langle u \rangle^+ (z;\xi) = (1+\boldsymbol{\epsilon}(z;\xi))U^+(z;\xi)$$

$$\left\langle \boldsymbol{\epsilon}(z)\boldsymbol{\epsilon}(z') \right\rangle = \sigma^2 \exp\left(-1/2\frac{(z-z')^2}{l^2}\right)$$

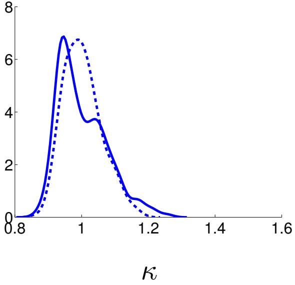


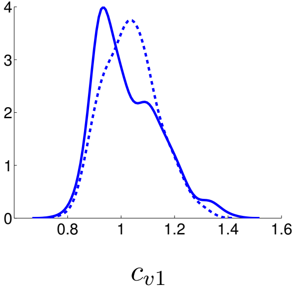
Numerical Results

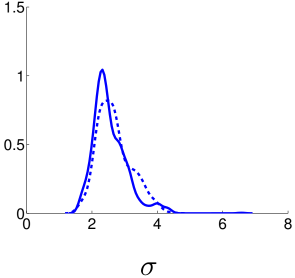
Correlated inhomogeneous covariance:

$$\langle u \rangle^+(z;\xi) = (1+\boldsymbol{\epsilon}(z;\xi))U^+(z;\xi)$$

$$\langle \boldsymbol{\epsilon}(z)\boldsymbol{\epsilon}(z') \rangle = \sigma^2 \left(\frac{2l(z)l(z')}{l^2(z)+l^2(z')} \right)^{1/2} \exp\left(-\frac{(z-z')^2}{l^2(z)+l^2(z')} \right)$$





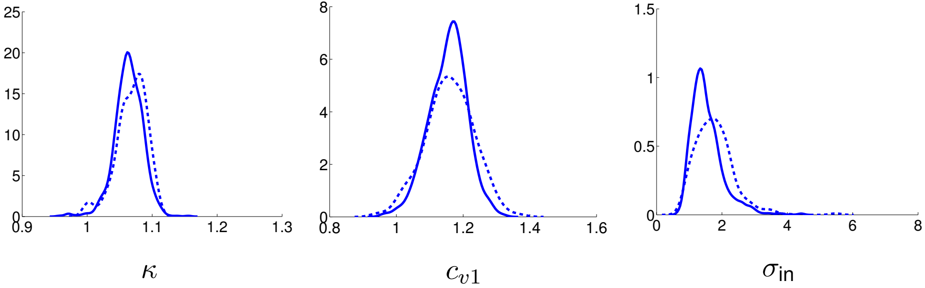


Numerical Results

Reynolds stress uncertainty:

$$\left\langle \boldsymbol{u}_i' \boldsymbol{u}_j' \right\rangle^+ (z;\xi) = T^+(z;\xi) - \boldsymbol{\epsilon}(z;\xi)$$
$$\left\langle \boldsymbol{\epsilon}(z)\boldsymbol{\epsilon}(z') \right\rangle = k_{\text{in}}(z,z') + k_{\text{out}}(z,z')$$

where k_{in} models the error near the walls and k_{out} far from the walls.



Numerical Results: Model selection

Model evidence ($\log(E)$):

	Surrogate	Full model
Independent homogeneous	-1.457	8.862
Correlated homogeneous	1.963	8.045
Correlated inhomogeneous	164.9	164.0
Reynolds stress	164.8	169.0

Relative runtimes (in seconds):

	Surrogate	Full model
Independent homogeneous	130	1720
Correlated homogeneous	162	1906
Correlated inhomogeneous	151	1735
Reynolds stress	147	1743
Cumulative	590	7104

Concluding remarks and future work

- We need to think about errors and error control in computational science and engineering. We need quantitative methods to assess the reliability of our predictions (with respect to a given goal).
- Formulation of the problem should be done with respect to the goal of the computation, not necessarily by minimizing the energy of the system.